SUPPORTING INFORMATIONS

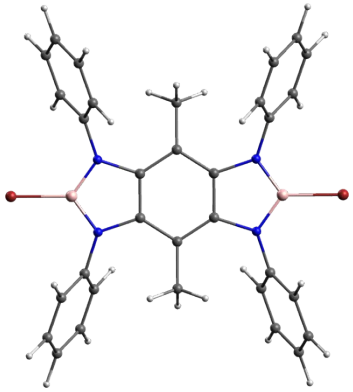
Syntheses and Structures of Benzobis(1,3,2-diazaboroles) and Acenaphtho-1,3,2 – diazaboroles

Lothar Weber* [a]Daniel Eickhoff [a] Chrostowska [b], Alain Dargelos [b] Clovis Darrigan [b] Hans-Georg Stammler [a] and Beate Neumann[a]

[a] Fakultät für Chemie der Universität Bielefeld, 33615 Bielefeld, Germany.
E-mail: lothar.weber@uni-bielefeld.de

[b] Université de Pau et des Pays de l'Adour / E2S UPPA, Institut des Sciences Analytiques et de Physico-Chimie pour l'Environnement et les Matériaux, UMR5254, 64000 Pau, France.
E-mail: anna.chrostowska@univ-pau.fr

1. Compound 4



Neutral, ground state, CAM-B3LYP/6-311G(d,p)

Atomic coordinates of optimized geometry
C_{2h} symmetry

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	0.000000	0.000000	5.276417
2	7	-1.138431	0.172450	2.519335
3	7	1.138431	-0.172450	2.519335
4	5	0.000000	0.000000	3.352782
5	6	-0.694361	0.116467	1.174816
6	6	0.694361	-0.116467	1.174816
7	6	1.427769	-0.294707	0.000000
8	6	2.859200	-0.767679	0.000000
9	1	3.058812	-1.378335	-0.877281
10	1	3.058812	-1.378335	0.877281
11	1	3.583636	0.049204	0.000000
12	6	-2.496140	0.073734	2.946666
13	6	-3.237191	-1.066170	2.657004
14	1	-2.778563	-1.865007	2.086730
15	6	-4.547589	-1.171138	3.096092
16	1	-5.121022	-2.061040	2.865708
17	6	-5.120064	-0.147128	3.838616
18	1	-6.142909	-0.232423	4.184626
19	6	-4.373876	0.982538	4.140708
20	1	-4.811536	1.782963	4.724909
21	6	-3.065127	1.095791	3.694405
22	1	-2.476386	1.975727	3.920248
23	6	2.496140	-0.073734	2.946666
24	6	3.065127	-1.095791	3.694405
25	1	2.476386	-1.975727	3.920248
26	6	4.373876	-0.982538	4.140708
27	1	4.811536	-1.782963	4.724909
28	6	5.120064	0.147128	3.838616
29	1	6.142909	0.232423	4.184626
30	6	4.547589	1.171138	3.096092
31	1	5.121022	2.061040	2.865708
32	6	3.237191	1.066170	2.657004
33	1	2.778563	1.865007	2.086730
34	35	0.000000	0.000000	-5.276417
35	7	1.138431	-0.172450	-2.519335
36	7	-1.138431	0.172450	-2.519335
37	5	0.000000	0.000000	-3.352782
38	6	0.694361	-0.116467	-1.174816
39	6	-0.694361	0.116467	-1.174816
40	6	-1.427769	0.294707	0.000000
41	6	-2.859200	0.767679	0.000000
42	1	-3.058812	1.378335	0.877281
43	1	-3.058812	1.378335	-0.877281
44	1	-3.583636	-0.049204	0.000000
45	6	2.496140	-0.073734	-2.946666
46	6	3.237191	1.066170	-2.657004
47	1	2.778563	1.865007	-2.086730
48	6	4.547589	1.171138	-3.096092
49	1	5.121022	2.061040	-2.865708
50	6	5.120064	0.147128	-3.838616
51	1	6.142909	0.232423	-4.184626
52	6	4.373876	-0.982538	-4.140708

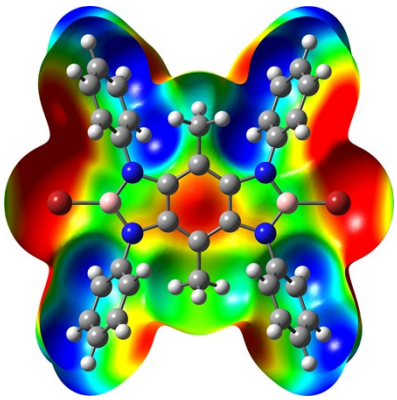
53	1	4.811536	-1.782963	-4.724909
54	6	3.065127	-1.095791	-3.694405
55	1	2.476386	-1.975727	-3.920248
56	6	-2.496140	0.073734	-2.946666
57	6	-3.065127	1.095791	-3.694405
58	1	-2.476386	1.975727	-3.920248
59	6	-4.373876	0.982538	-4.140708
60	1	-4.811536	1.782963	-4.724909
61	6	-5.120064	-0.147128	-3.838616
62	1	-6.142909	-0.232423	-4.184626
63	6	-4.547589	-1.171138	-3.096092
64	1	-5.121022	-2.061040	-2.865708
65	6	-3.237191	-1.066170	-2.657004
66	1	-2.778563	-1.865007	-2.086730

SCF Energy of neutral: -6652.025172460000 au
Dipole moment (Debye):
x= 0.000 y= 0.000 z= 0.000 Norm= 0.000

HOMO = -6.550 eV LUMO = 0.695 eV gap(HOMO-LUMO) = 7.245 eV

MO	(#)	au	eV
LUMO+4	(168)	0.02997	0.8155
LUMO+3	(167)	0.02977	0.8101
LUMO+2	(166)	0.02887	0.7856
LUMO+1	(165)	0.02701	0.7350
LUMO	(164)	0.02553	0.6947
HOMO	(163)	-0.24072	-6.5503
HOMO-1	(162)	-0.25425	-6.9185
HOMO-2	(161)	-0.30201	-8.2181
HOMO-3	(160)	-0.30528	-8.3071
HOMO-4	(159)	-0.30741	-8.3651
HOMO-5	(158)	-0.31480	-8.5661
HOMO-6	(157)	-0.31536	-8.5814
HOMO-7	(156)	-0.31655	-8.6138
HOMO-8	(155)	-0.31844	-8.6652
HOMO-9	(154)	-0.31883	-8.6758
Gap (au ; eV ; nm)		0.26625 ;	7.2450 ;	171.13

Electrostatic Potential Surface Map at the 0.001 electron.bohr^{-3} density iso-contour level (from +12.55 to -12.55 kcal/mol); red = negative charge; blue = positive charge.



Cation, ground state, CAM-B3LYP/6-311G(d,p)

SCF Energy of cation: -6651.779710660000 au
First IE Delta-SCF: 6.6794 eV

Neutral, ground state, CAM-B3LYP/6-311++G(d,p)

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SCF Energy of neutral:    -6652.038147250000       au
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Anion, ground state, CAM-B3LYP/6-311G++(d,p)

```
SCF Energy of anion:    -6652.022085330000      au
First EA Delta-SCF:  -0.4371 eV
(With EA = E(M) - E(M-) by convention)
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Gap Δ_{IE-EA} = 7.1165 eV

Neutral, first excited state, TD-CAM-B3LYP/6-311G(d,p)

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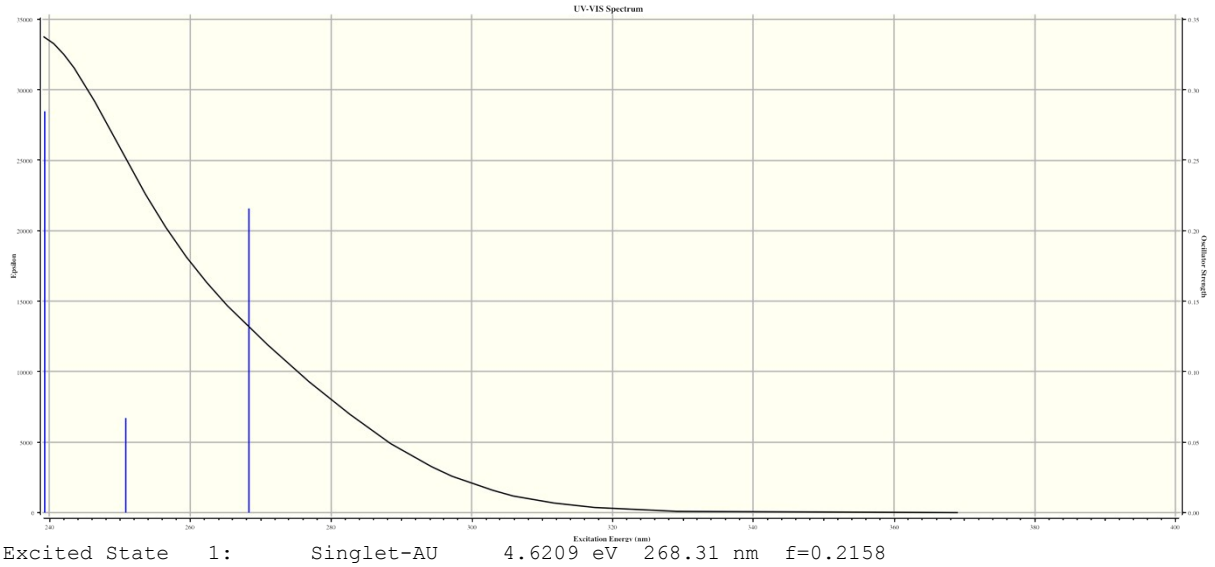
Dipole moment of excited state (Debye):
    x=   0.000   y=   0.000   z=   0.000   Norm=   0.000

Vectorial difference between dipole moments excited-fundamental:
    x=   0.000   y=   0.000   z=   0.000   Norm=   0.000
```

Neutral at ground state geometry, UV-visible spectrum TD-CAM-B3LYP/6-311G(d,p)

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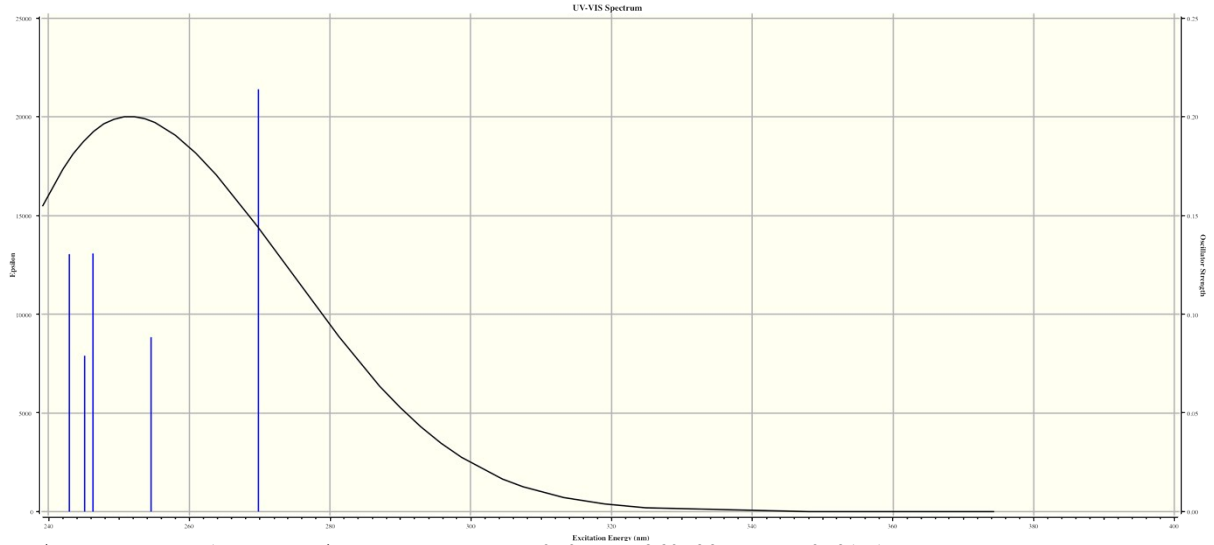
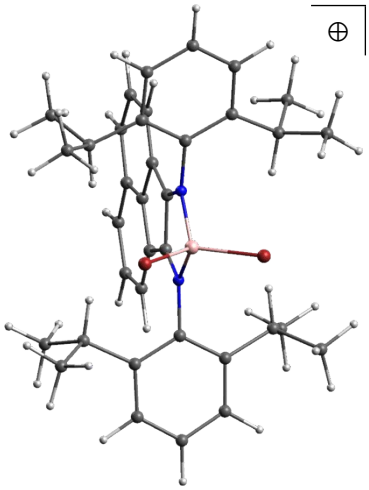
Excited State   1:      Singlet-AU     4.6209 eV  268.31 nm  f=0.2158
Excited State   2:      Singlet-BU     4.9427 eV  250.84 nm  f=0.0670
Excited State   3:      Singlet-BG     5.1022 eV  243.00 nm  f=0.0000
Excited State   4:      Singlet-AU     5.1812 eV  239.30 nm  f=0.2847
Excited State   5:      Singlet-BU     5.1977 eV  238.54 nm  f=0.1149
Excited State   6:      Singlet-AG     5.2041 eV  238.24 nm  f=0.0000
Excited State   7:      Singlet-AU     5.2183 eV  237.60 nm  f=0.0652
Excited State   8:      Singlet-BG     5.2328 eV  236.94 nm  f=0.0000
Excited State   9:      Singlet-AG     5.2942 eV  234.19 nm  f=0.0000
Excited State  10:      Singlet-BU     5.3502 eV  231.74 nm  f=0.3485
```

Neutral at ground state geometry, UV-visible spectrum TD-CAM-B3LYP/6-311++G(d,p)



Excited State	1:	Singlet-AU	4.5950 eV	269.82 nm	f=0.2141
Excited State	2:	Singlet-BG	4.7715 eV	259.85 nm	f=0.0000
Excited State	3:	Singlet-BU	4.8706 eV	254.56 nm	f=0.0883
Excited State	4:	Singlet-BG	5.0134 eV	247.30 nm	f=0.0000
Excited State	5:	Singlet-AU	5.0328 eV	246.35 nm	f=0.1307
Excited State	6:	Singlet-BU	5.0583 eV	245.11 nm	f=0.0789
Excited State	7:	Singlet-AG	5.0642 eV	244.82 nm	f=0.0000
Excited State	8:	Singlet-AG	5.0951 eV	243.34 nm	f=0.0000
Excited State	9:	Singlet-AU	5.1024 eV	242.99 nm	f=0.1305
Excited State	10:	Singlet-BG	5.1727 eV	239.69 nm	f=0.0000

2. Compound 6



Cation, ground state, CAM-B3LYP/6-311G(d,p)

Atomic coordinates of optimized geometry
C_{2v} symmetry

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	-1.623713	0.000000	-2.425423
2	35	1.623713	0.000000	-2.425423
3	7	0.000000	1.215983	-0.234703
4	7	0.000000	-1.215983	-0.234703
5	5	0.000000	0.000000	-1.295847
6	6	0.000000	0.743865	0.956945
7	6	0.000000	-0.743865	0.956945
8	6	0.000000	-1.196004	2.329877
9	6	0.000000	0.000000	3.098429
10	6	0.000000	1.196004	2.329877
11	6	0.000000	-2.414233	2.965751
12	1	0.000000	-3.342393	2.409664
13	6	0.000000	-2.428772	4.376701
14	1	0.000000	-3.383910	4.885511
15	6	0.000000	-1.270928	5.121267
16	1	0.000000	-1.329612	6.203416
17	6	0.000000	0.000000	4.492522
18	6	0.000000	1.270928	5.121267
19	1	0.000000	1.329612	6.203416
20	6	0.000000	2.428772	4.376701
21	1	0.000000	3.383910	4.885511
22	6	0.000000	2.414233	2.965751
23	1	0.000000	3.342393	2.409664
24	6	0.000000	2.656638	-0.478523
25	6	-1.233224	3.324009	-0.553773
26	6	-1.196140	4.697094	-0.778081
27	1	-2.128113	5.242192	-0.851368
28	6	0.000000	5.377634	-0.902972
29	1	0.000000	6.445224	-1.084969
30	6	1.196140	4.697094	-0.778081
31	1	2.128113	5.242192	-0.851368
32	6	1.233224	3.324009	-0.553773
33	6	-2.588672	2.664956	-0.344205
34	1	-2.450428	1.585867	-0.294528
35	6	-3.219354	3.116148	0.980503
36	1	-2.586810	2.880347	1.838441
37	1	-4.180862	2.619671	1.126980
38	1	-3.399869	4.193146	0.985415
39	6	-3.546651	2.940345	-1.508001
40	1	-4.462470	2.359548	-1.382090
41	1	-3.102163	2.670959	-2.465414
42	1	-3.832398	3.993135	-1.550288
43	6	2.588672	2.664956	-0.344205
44	1	2.450428	1.585867	-0.294528
45	6	3.219354	3.116148	0.980503
46	1	3.399869	4.193146	0.985415
47	1	4.180862	2.619671	1.126980
48	1	2.586810	2.880347	1.838441
49	6	3.546651	2.940345	-1.508001
50	1	3.102163	2.670959	-2.465414
51	1	4.462470	2.359548	-1.382090
52	1	3.832398	3.993135	-1.550288

53	6	0.000000	-2.656638	-0.478523
54	6	1.233224	-3.324009	-0.553773
55	6	1.196140	-4.697094	-0.778081
56	1	2.128113	-5.242192	-0.851368
57	6	0.000000	-5.377634	-0.902972
58	1	0.000000	-6.445224	-1.084969
59	6	-1.196140	-4.697094	-0.778081
60	1	-2.128113	-5.242192	-0.851368
61	6	-1.233224	-3.324009	-0.553773
62	6	2.588672	-2.664956	-0.344205
63	1	2.450428	-1.585867	-0.294528
64	6	3.219354	-3.116148	0.980503
65	1	2.586810	-2.880347	1.838441
66	1	4.180862	-2.619671	1.126980
67	1	3.399869	-4.193146	0.985415
68	6	3.546651	-2.940345	-1.508001
69	1	4.462470	-2.359548	-1.382090
70	1	3.102163	-2.670959	-2.465414
71	1	3.832398	-3.993135	-1.550288
72	6	-2.588672	-2.664956	-0.344205
73	1	-2.450428	-1.585867	-0.294528
74	6	-3.219354	-3.116148	0.980503
75	1	-3.399869	-4.193146	0.985415
76	1	-4.180862	-2.619671	1.126980
77	1	-2.586810	-2.880347	1.838441
78	6	-3.546651	-2.940345	-1.508001
79	1	-3.832398	-3.993135	-1.550288
80	1	-3.102163	-2.670959	-2.465414
81	1	-4.462470	-2.359548	-1.382090

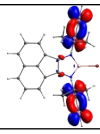
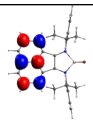
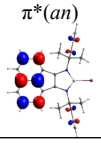
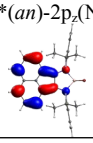
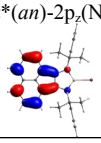
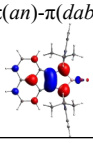
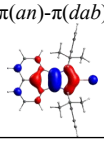
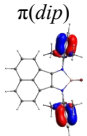
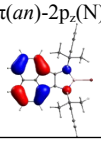
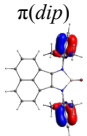
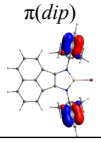
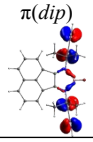
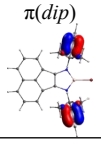
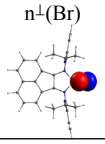
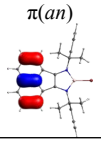
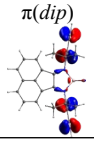
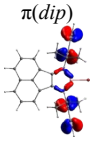
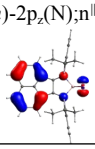
SCF Energy of cation: -6678.166133450000 au

HOMO = -10.819 eV LUMO = -5.839 eV gap(HOMO-LUMO) = 4.980 eV

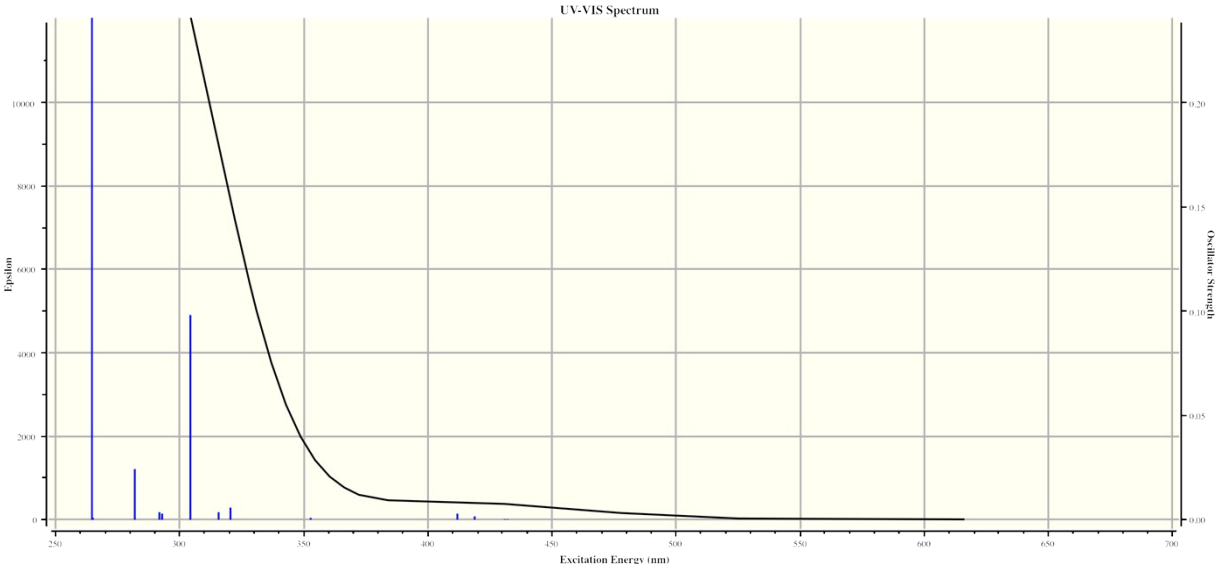
MO	(#)	au	eV
LUMO+4	(177)	-0.06855	-1.8653
LUMO+3	(176)	-0.07419	-2.0188
LUMO+2	(175)	-0.11474	-3.1222
LUMO+1	(174)	-0.18059	-4.9141
LUMO	(173)	-0.21458	-5.8390
HOMO	(172)	-0.39759	-10.8190
HOMO-1	(171)	-0.39787	-10.8266
HOMO-2	(170)	-0.41406	-11.2671
HOMO-3	(169)	-0.41581	-11.3148
HOMO-4	(168)	-0.41637	-11.3300
HOMO-5	(167)	-0.41928	-11.4092
HOMO-6	(166)	-0.43638	-11.8745
HOMO-7	(165)	-0.44768	-12.1820
HOMO-8	(164)	-0.44821	-12.1964
HOMO-9	(163)	-0.45032	-12.2538
Gap (au ; eV ; nm)		0.18301 ;	4.9800 ; 248.97

Molecular orbitals comparison of intermediate **6** (cationic part only) with final product **7**:
(*dab*: diazaborole; *dip*: 2,5-di(isopropyl)phenyl; *an*: acenaphthylen)

	7 (C_{2v})	**6** (C_{2v})
LUMO+2	0.9323 (a_2) π^*(*dip*)	-3.1222 (b_1) π^*(*an*)

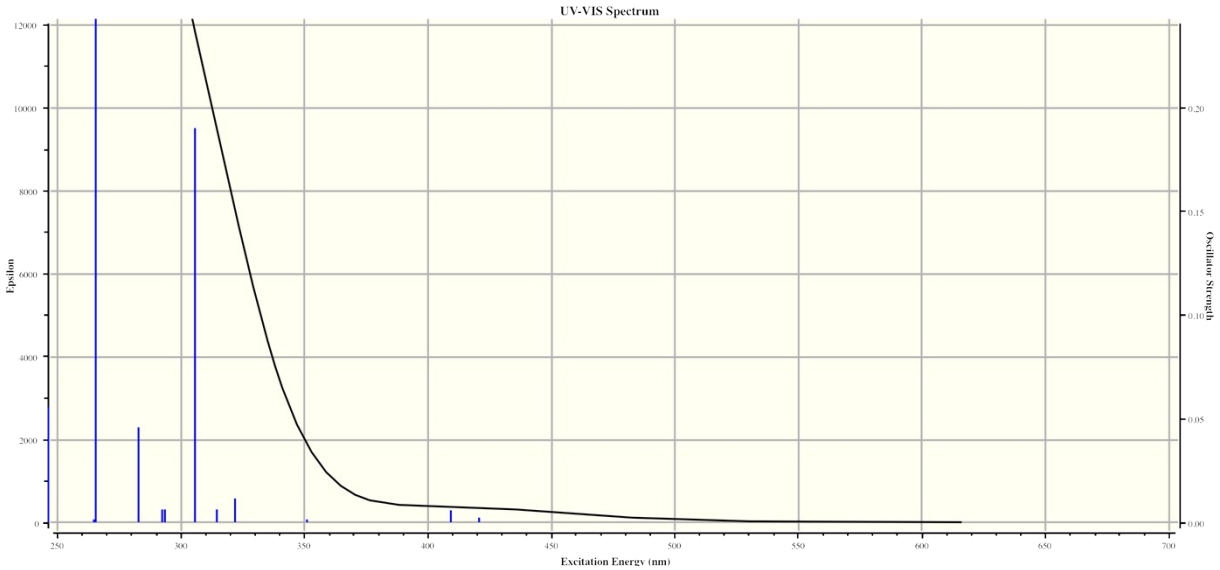
		
LUMO+1	0.6547 (b_1) π^*(*an*) 	-4.9141 (a_2) π^*(*an*)-2p_z(N) 
LUMO	-0.8751 (a_2) π^*(*an*)-2p_z(N) 	-5.8390 (b_1) π(*an*)-π(*dab*) 
HOMO	-6.5003 (b_1) π(*an*)-π(*dab*) 	-10.8190 (a_2) π(*dip*) 
HOMO-1	-7.6461 (a_2) π(*an*)-2p_z(N) 	-10.8266 (b_2) π(*dip*) 
HOMO-2	-8.0788 (b_2) π(*dip*) 	-11.2671 (a_1) π(*dip*) 
HOMO-3	-8.0910 (a_1) π(*dip*) 	-11.3148 (b_1) $n^{\perp}$(Br) 
HOMO-4	-8.2851 (b_1) π(*an*) 	-11.3300 (a_2) π(*dip*) 
HOMO-5	-8.2867 (a_2) π(*dip*) 	-11.4092 (b_1) π(*an*)-2p_z(N);$n^{\parallel}$(Br) 

Cation at ground state geometry, UV-visible spectrum TD-CAM-B3LYP/6-311G(d,p)




```
Excited State   1:      Singlet-B2     2.8695 eV  432.07 nm  f=0.0003
Excited State   2:      Singlet-A1     2.8767 eV  431.00 nm  f=0.0003
Excited State   3:      Singlet-A2     2.9542 eV  419.69 nm  f=0.0000
Excited State   4:      Singlet-B2     2.9600 eV  418.87 nm  f=0.0031
Excited State   5:      Singlet-A1     3.0112 eV  411.74 nm  f=0.0057
Excited State   6:      Singlet-B1     3.0185 eV  410.74 nm  f=0.0002
Excited State   7:      Singlet-B2     3.5157 eV  352.65 nm  f=0.0018
Excited State   8:      Singlet-A2     3.7622 eV  329.55 nm  f=0.0000
Excited State   9:      Singlet-A1     3.8682 eV  320.52 nm  f=0.0116
Excited State  10:      Singlet-B1     3.9278 eV  315.65 nm  f=0.0069
Excited State  11:      Singlet-A1     4.0761 eV  304.17 nm  f=0.1928
Excited State  12:      Singlet-B2     4.2344 eV  292.80 nm  f=0.0059
Excited State  13:      Singlet-A1     4.2466 eV  291.96 nm  f=0.0070
Excited State  14:      Singlet-B2     4.3971 eV  281.97 nm  f=0.0478
Excited State  15:      Singlet-B1     4.5454 eV  272.77 nm  f=0.0000
Excited State  16:      Singlet-A2     4.5978 eV  269.66 nm  f=0.0000
Excited State  17:      Singlet-B2     4.6771 eV  265.09 nm  f=0.0017
Excited State  18:      Singlet-A1     4.6876 eV  264.49 nm  f=0.5714
Excited State  19:      Singlet-B2     5.0408 eV  245.96 nm  f=0.0549
Excited State  20:      Singlet-A2     5.0737 eV  244.37 nm  f=0.0000
```

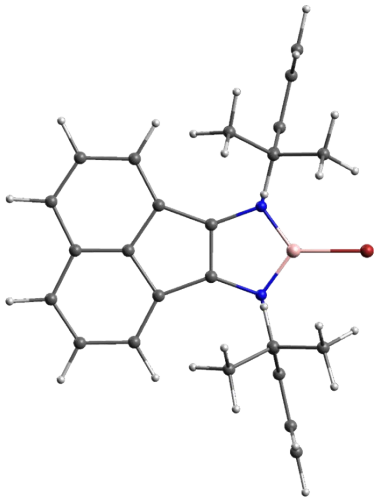
Cation at ground state geometry, UV-visible spectrum TD-CAM-B3LYP/6-311G++(d,p)




```
Excited State   1:      Singlet-B2     2.8715 eV  431.77 nm  f=0.0004
Excited State   2:      Singlet-A1     2.8821 eV  430.19 nm  f=0.0002
Excited State   3:      Singlet-B2     2.9476 eV  420.63 nm  f=0.0026
Excited State   4:      Singlet-A2     2.9586 eV  419.06 nm  f=0.0000
Excited State   5:      Singlet-B1     3.0229 eV  410.15 nm  f=0.0002
Excited State   6:      Singlet-A1     3.0285 eV  409.39 nm  f=0.0058
Excited State   7:      Singlet-B2     3.5327 eV  350.96 nm  f=0.0015
```

Excited State	8:	Singlet-A2	3.7801 eV	327.99 nm	f=0.0000
Excited State	9:	Singlet-A1	3.8529 eV	321.79 nm	f=0.0117
Excited State	10:	Singlet-B1	3.9420 eV	314.52 nm	f=0.0065
Excited State	11:	Singlet-A1	4.0577 eV	305.55 nm	f=0.1904
Excited State	12:	Singlet-B2	4.2262 eV	293.37 nm	f=0.0064
Excited State	13:	Singlet-A1	4.2397 eV	292.44 nm	f=0.0065
Excited State	14:	Singlet-B2	4.3854 eV	282.72 nm	f=0.0462
Excited State	15:	Singlet-B1	4.5381 eV	273.21 nm	f=0.0000
Excited State	16:	Singlet-A2	4.5907 eV	270.08 nm	f=0.0000
Excited State	17:	Singlet-A1	4.6737 eV	265.28 nm	f=0.5690
Excited State	18:	Singlet-B2	4.6822 eV	264.80 nm	f=0.0015
Excited State	19:	Singlet-B2	5.0381 eV	246.09 nm	f=0.0555
Excited State	20:	Singlet-A2	5.0725 eV	244.43 nm	f=0.0000

3. Compound 7



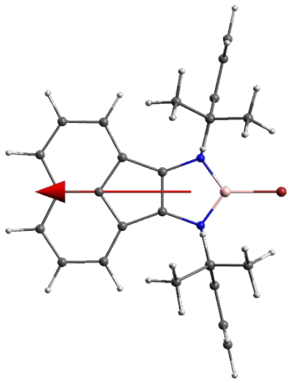
Neutral, ground state, CAM-B3LYP/6-311G(d,p)

Atomic coordinates of optimized geometry
C_{2v} symmetry

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	35	0.000000	0.000000	3.092110
2	7	0.000000	1.156840	0.323796
3	7	0.000000	-1.156840	0.323796
4	5	0.000000	0.000000	1.166819
5	6	0.000000	0.680452	-0.983143
6	6	0.000000	-0.680452	-0.983143
7	6	0.000000	-1.180889	-2.356461
8	6	0.000000	0.000000	-3.152012
9	6	0.000000	1.180889	-2.356461
10	6	0.000000	2.392643	-2.991390
11	1	0.000000	3.324741	-2.439368
12	6	0.000000	2.416994	-4.413647
13	1	0.000000	3.380075	-4.910204
14	6	0.000000	1.273957	-5.170218
15	1	0.000000	1.336717	-6.252421
16	6	0.000000	0.000000	-4.536090
17	6	0.000000	-1.273957	-5.170218
18	1	0.000000	-1.336717	-6.252421
19	6	0.000000	-2.416994	-4.413647
20	1	0.000000	-3.380075	-4.910204
21	6	0.000000	-2.392643	-2.991390
22	1	0.000000	-3.324741	-2.439368
23	6	0.000000	2.551877	0.651159
24	6	-1.224100	3.217776	0.798921
25	6	-1.197531	4.575484	1.103056
26	1	-2.131253	5.111229	1.225663
27	6	0.000000	5.251046	1.254029
28	1	0.000000	6.308153	1.492648
29	6	1.197531	4.575484	1.103056
30	1	2.131253	5.111229	1.225663
31	6	1.224100	3.217776	0.798921
32	6	-2.558403	2.509159	0.643238
33	1	-2.355058	1.466111	0.399685
34	6	-3.356021	2.528552	1.951747
35	1	-2.785148	2.083303	2.768363
36	1	-4.285667	1.965390	1.838460
37	1	-3.619628	3.548698	2.242146
38	6	-3.376652	3.096118	-0.511876
39	1	-3.635689	4.141635	-0.326896
40	1	-4.309259	2.540726	-0.636884
41	1	-2.825661	3.046739	-1.452971
42	6	2.558403	2.509159	0.643238
43	1	2.355058	1.466111	0.399685
44	6	3.356021	2.528552	1.951747
45	1	3.619628	3.548698	2.242146
46	1	4.285667	1.965390	1.838460
47	1	2.785148	2.083303	2.768363
48	6	3.376652	3.096118	-0.511876
49	1	2.825661	3.046739	-1.452971
50	1	4.309259	2.540726	-0.636884
51	1	3.635689	4.141635	-0.326896
52	6	0.000000	-2.551877	0.651159

53	6	-1.224100	-3.217776	0.798921
54	6	-1.197531	-4.575484	1.103056
55	1	-2.131253	-5.111229	1.225663
56	6	0.000000	-5.251046	1.254029
57	1	0.000000	-6.308153	1.492648
58	6	1.197531	-4.575484	1.103056
59	1	2.131253	-5.111229	1.225663
60	6	1.224100	-3.217776	0.798921
61	6	-2.558403	-2.509159	0.643238
62	1	-2.355058	-1.466111	0.399685
63	6	-3.376652	-3.096118	-0.511876
64	1	-2.825661	-3.046739	-1.452971
65	1	-4.309259	-2.540726	-0.636884
66	1	-3.635689	-4.141635	-0.326896
67	6	-3.356021	-2.528552	1.951747
68	1	-3.619628	-3.548698	2.242146
69	1	-4.285667	-1.965390	1.838460
70	1	-2.785148	-2.083303	2.768363
71	6	2.558403	-2.509159	0.643238
72	1	2.355058	-1.466111	0.399685
73	6	3.356021	-2.528552	1.951747
74	1	2.785148	-2.083303	2.768363
75	1	4.285667	-1.965390	1.838460
76	1	3.619628	-3.548698	2.242146
77	6	3.376652	-3.096118	-0.511876
78	1	3.635689	-4.141635	-0.326896
79	1	4.309259	-2.540726	-0.636884
80	1	2.825661	-3.046739	-1.452971

SCF Energy of neutral: -4104.146037500000 au
Dipole moment (Debye):
x = 0.000 y = 0.000 z = -1.793 Norm = 1.793

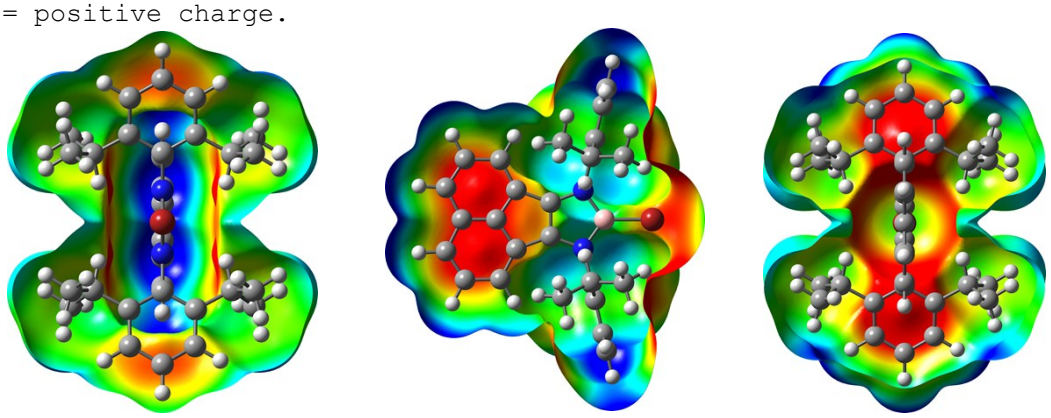


HOMO = -6.500 eV LUMO = -0.875 eV gap(HOMO-LUMO) = 5.625 eV

MO	(#)	au	eV
LUMO+4	(160)	0.03702	1.0074
LUMO+3	(159)	0.03452	0.9393
LUMO+2	(158)	0.03426	0.9323
LUMO+1	(157)	0.02406	0.6547
LUMO	(156)	-0.03216	-0.8751
HOMO	(155)	-0.23888	-6.5003
HOMO-1	(154)	-0.28099	-7.6461
HOMO-2	(153)	-0.29689	-8.0788
HOMO-3	(152)	-0.29734	-8.0910
HOMO-4	(151)	-0.30447	-8.2851
HOMO-5	(150)	-0.30453	-8.2867
HOMO-6	(149)	-0.30820	-8.3865

```
HOMO-7   (148)   -0.34738    -9.4527
HOMO-8   (147)   -0.34804    -9.4707
HOMO-9   (146)   -0.34828    -9.4772
Gap (au ; eV ; nm)          0.20672 ;     5.6251 ;     220.41
```

Electrostatic Potential Surface Map at the 0.001 electron.bohr^{-3} density iso-contour level (from +12.55 to -12.55 kcal/mol); red = negative charge; blue = positive charge.



Cation, ground state, CAM-B3LYP/6-311G(d,p)

```
SCF Energy of cation:     -4103.904016190000       au
First IE Delta-SCF:    6.5857 eV
```

Neutral, ground state, CAM-B3LYP/6-311++G(d,p)

```
SCF Energy of neutral:     -4104.156485680000        au
```

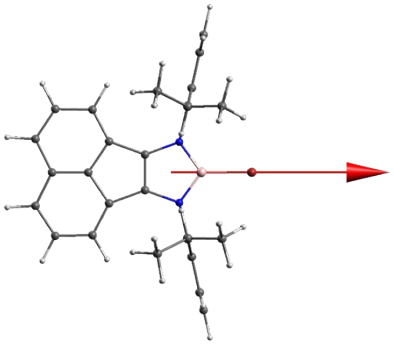
Anion, ground state, CAM-B3LYP/6-311G++(d,p)

```
SCF Energy of anion:     -4104.181692410000       au
First EA Delta-SCF:    0.6859 eV
(With EA = E(M) - E(M-) by convention)
```

Gap Δ_{IE-EA} = 5.8998 eV

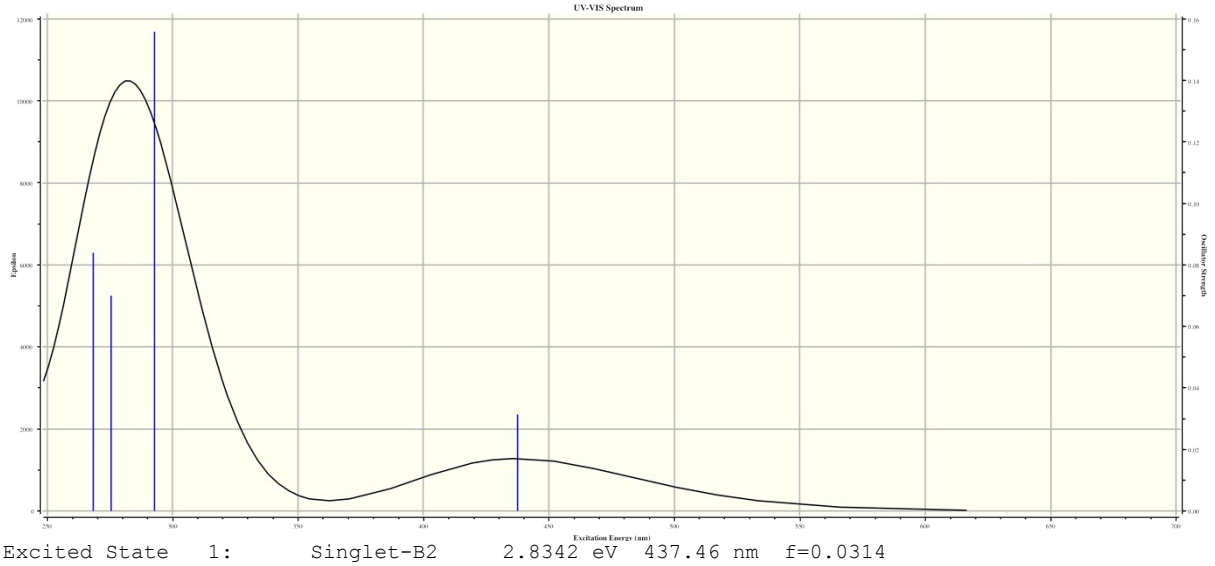
Neutral, first excited state, TD-CAM-B3LYP/6-311G(d,p)

```
Dipole moment of excited state (Debye):
    x =    0.000    y =    0.000    z =    2.796    Norm =    2.796
```



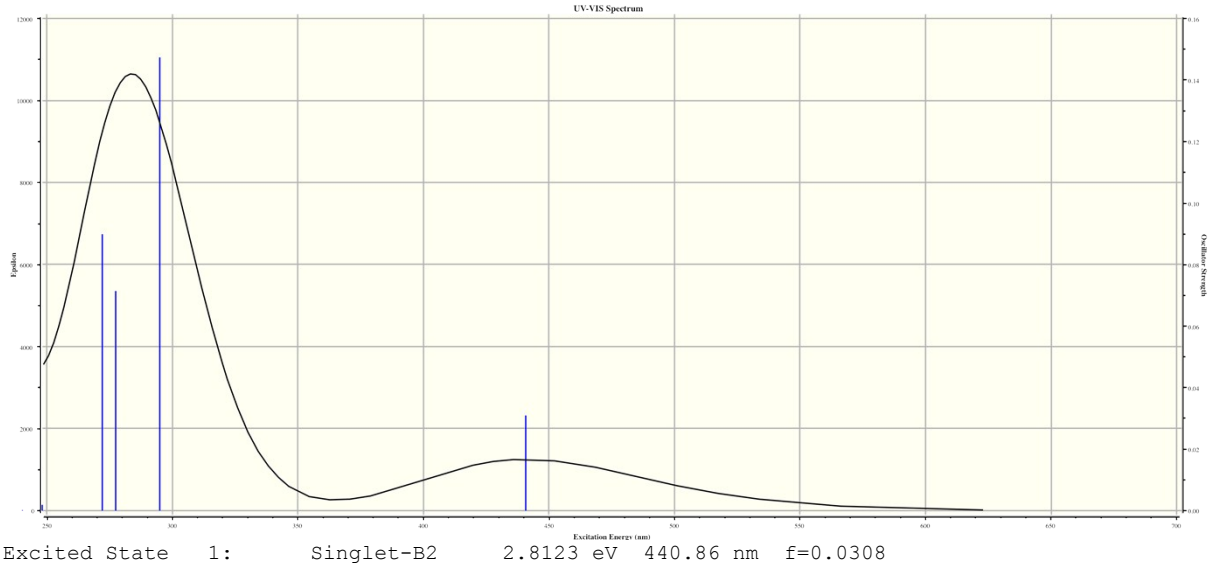
```
Vectorial difference between dipole moments excited-fundamental:
    x =    0.000    y =    0.000    z =    4.589    Norm =    4.589
```

Neutral at ground state geometry, UV-visible spectrum TD-CAM-B3LYP/6-311G(d,p)



Excited State	1:	Singlet-B2	2.8342 eV	437.46 nm	f=0.0314
Excited State	2:	Singlet-A1	4.2348 eV	292.78 nm	f=0.1558
Excited State	3:	Singlet-B2	4.5014 eV	275.43 nm	f=0.0700
Excited State	4:	Singlet-A1	4.6202 eV	268.35 nm	f=0.0840
Excited State	5:	Singlet-B1	5.1937 eV	238.72 nm	f=0.0000
Excited State	6:	Singlet-A2	5.3598 eV	231.32 nm	f=0.0000
Excited State	7:	Singlet-B2	5.3749 eV	230.67 nm	f=0.0057
Excited State	8:	Singlet-A1	5.3787 eV	230.51 nm	f=0.0460
Excited State	9:	Singlet-B1	5.4044 eV	229.41 nm	f=0.0050
Excited State	10:	Singlet-A2	5.4118 eV	229.10 nm	f=0.0000

Neutral at ground state geometry, UV-visible spectrum TD-CAM-B3LYP/6-311++G(d,p)

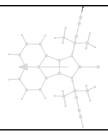
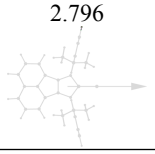


Excited State	1:	Singlet-B2	2.8123 eV	440.86 nm	f=0.0308
Excited State	2:	Singlet-A1	4.2009 eV	295.13 nm	f=0.1473
Excited State	3:	Singlet-B2	4.4701 eV	277.36 nm	f=0.0714
Excited State	4:	Singlet-A1	4.5572 eV	272.06 nm	f=0.0899
Excited State	5:	Singlet-B1	4.9931 eV	248.31 nm	f=0.0018
Excited State	6:	Singlet-B1	5.1599 eV	240.29 nm	f=0.0001
Excited State	7:	Singlet-B2	5.2905 eV	234.35 nm	f=0.0062
Excited State	8:	Singlet-A1	5.2930 eV	234.24 nm	f=0.0652
Excited State	9:	Singlet-A2	5.3200 eV	233.05 nm	f=0.0000
Excited State	10:	Singlet-B1	5.3648 eV	231.10 nm	f=0.0026

Summary table for compounds 4 and 7

[CAM-B3LYP/6-311G(d,p)] Calculated MO energies ε^{KS} (LUMO+2 to HOMO-3), plotted at ±0.04 isovalue, HOMO-LUMO gap ($\Delta_{H\text{-}L}$), gap $\Delta_{IE\text{-}EA}$, dipole moments for ground (μ_0) and first excited (μ_1) states, norm of vectorial difference ($||\Delta\boldsymbol{\mu}||=||\boldsymbol{\mu}_1\text{-}\boldsymbol{\mu}_0||$), difference of norms ($\Delta\mu=\mu_1\text{-}\mu_0$), first four ΔSCF+TD-DFT ionization energies, first UV-visible transition λ_1 [λ_1^{++}] from TD-DFT/CAM-B3LYP calculation 6-311G(d,p) [6-311++G(d,p)]. Subscript "ex" stands for vertical excitation from ground state. Element (color): H (white), B (light pink), C (grey), N (dark blue), N (dark red); *ph*: phenyl; *xy*: xylyl; *dab*: diazaborole; *dip*: 2,5-di(isopropyl)phenyl; *an*: acenaphthylen.

	7 (C_{2v})	**4** (C_{2h})
LUMO+2	0.9323 (a_2) π*(*dip*)	0.7856 (a_g) π*(*ph*);2p_z(B);π*(xy)
LUMO+1	0.6547 (b_1) π*(*an*)	0.7350 (b_g) π*(*ph*)
LUMO	-0.8751 (a_2) π*(*an*)-2p_z(N)	0.6947 (a_u) π*(*ph*);π*(*xy*)
HOMO	-6.5003 (b_1) π(*an*)-π(*dab*)	-6.5503 (b_g) π(*xy*)-π(*dab*)
HOMO-1	-7.6461 (a_2) π(*an*)-2p_z(N)	-6.9185 (a_g) π(*xy*)-2p_z(N)
HOMO-2	-8.0788 (b_2) π(*dip*)	-8.2181 (a_u) σ(*ph*)-σ(*dab*)
HOMO-3	-8.0910 (a_1) π(*dip*)	-8.3071 (b_u) σ(*ph*)-σ(*dab*)
$\Delta_{H\text{-}L}$ (eV)	5.625	7.245
$\Delta_{IE\text{-}EA}$ (eV)	5.900	7.117
μ_0 (D)	1.793	0.000 —

		
μ_1 (D)	2.796 	0.000 —
$\|\|\Delta\boldsymbol{\mu}\|\|$ (D)	4.589	(0.000)
$\Delta\mu$ (D)	1.003	(0.000)
EI_1 (eV)	6.59	6.68
EI_2 (eV)	8.04	7.16
EI_3 (eV)	8.67	8.63
EI_4 (eV)	8.68	8.78
$\lambda_{1,ex}$ (eV, *nm*)	2.834 *438*	4.621 *251*
$\lambda_{1,ex}^{++}$ (eV, *nm*)	2.812 *441*	4.621 *268*